IR SPECTROSCOPIC STUDY ON PHENOL-TRIETHYLSILANE DIHYDROGEN-BONDED CLUSTER IN THE ELECTRONIC EXCITED STATE

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To reveal detailed characters of the dihydrogen bond at molecular level, we have been carrying out IR spectroscopic study on the Si-H$\cdots$H-O type dihydrogen-bonded clusters[a,b]. It was found that the structures of the phenol-alkylsilane 1:1 clusters are determined by the competition between the dihydrogen bond and the dispersion interaction in the case of the S_0 state of the neutral clusters. On the other hand, the dihydrogen bond exhibit a dominant contribution in the cationic states. Based on these results, it is expected the balance between the dihydrogen bond and the dispersion interaction is expected to change in the S_1 state compared with the S_0 state. Thus, we have carried out an IR spectroscopic study on the phenol-alkylsilane clusters, in the present study.

In the present paper, we will report mainly on the results of the phenol-triethylsilane (PhOH-TES) clusters. It is already reported that three isomers appear in the fluorescence excitation spectrum of PhOH-TES. Using the vibronic bands of these isomers as excitation transitions, IR spectra in the S_1 state were observed by the UV-IR double resonance technique. All of the isomers exhibit much larger redshifts of the OH stretching band compared with those in the S_0 state. It indicates the strengthening of the dihydrogen bond in the S_1 state. In addition, all the isomer exhibit Franck-Condon-like patterns. The patterns change by the intermediate vibrational levels selected by the UV transitions. Similar Franck-Condon-like pattern in the IR transition is reported in the literature[c]. This result indicates a strong coupling between the OH stretch and the intermolecular vibrational mode. This coupling is considered to be a characteristic feature in the S_1 state.

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